Multiphysics Modeling of Pollutant Uptake by Mangroves

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Abstract: Metal contaminants and organic pollutants are affecting aquatic environments in urban and industrial zones. Mangrove trees are capable of absorbing metal ions and organic pollutants like PCB and PAH. Located in tidal zones of river estuaries mangrove forests may function as a means for immobilization and removal of pollutants. To estimate the remediation potential, two and three dimensional models of water and substance flow in the soil plant system based on porous media equations and on plant architecture are set up which is based on cohesion-tension theory. Water transport in soil and tree is conceived as a continuous hydraulic process, which is driven by canopy transpiration. State variables are water potential and contaminant concentrations in the soil, roots, xylem, core and canopy. The model equations are obtained by application of Richards equations with Mualem Van-Genuchten approaches for hydraulic conductivity and water retention specific for each plant compartment. The water transport equations are coupled to the contaminant transport equations via the Darcy velocity and the dispersion tensor. Exchanges between compartments are mediated by a diffusion model on the boundary for transport across membranes. Water evaporation from leaf mesophyll cells is taken into account by a transpiration sub model, which is driven by environmental variables such as air water potential, wind speed, radiation and temperature. Boundary conditions at the soil surface are subject to periodical tidal inundations by water with contaminant loads. This typical multiphysics problem couples physical and biological processes. The governing equations consist of a system of coupled non linear partial differential equations with reaction terms in two and three dimensions resp. which were implemented into the finite element tool COMSOL MULTIPHYSICS based on the Petrov-Galerkin scheme. Geometry models were generated in MATLAB and imported to COMSOL. Because of the extremely high differences in water potential between air and canopy and the strongly non linear character of the governing equations, boundary and initial conditions and net sizes and net structure have to be set up very carefully in order to achieve convergence. The model responses to changing environmental conditions -wind speed, inundations, photosynthetic active radiation, humidity of the air- in a reasonable way. For model validation experiments with young mangrove plants exposed to pollutants of different loads have been performed. First results show that the model is capable of reproducing typical spatial concentration patterns of metals in the plant.

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